A generative model for inorganic materials design

Abstract

The design of functional materials with desired properties is essential in driving technological advances in areas such as energy storage, catalysis and carbon capture1, 2–3. Generative models accelerate materials design by directly generating new materials given desired property constraints, but current methods have a low success rate in proposing stable crystals or can satisfy only a limited set of property constraints4, 5, 6, 7, 8, 9, 10–11. Here we present MatterGen, a model that generates stable, diverse inorganic materials across the periodic table and can further be fine-tuned to steer the generation towards a broad range of property constraints. Compared with previous generative models4,12, structures produced by MatterGen are more than twice as likely to be new and stable, and more than ten times closer to the local energy minimum. After fine-tuning, MatterGen successfully generates stable, new materials with desired chemistry, symmetry and mechanical, electronic and magnetic properties. As a proof of concept, we synthesize one of the generated structures and measure its property value to be within 20% of our target. We believe that the quality of generated materials and the breadth of abilities of MatterGen represent an important advancement towards creating a foundational generative model for materials design. MatterGen is a model that generates stable, diverse inorganic materials across the periodic table and can further be fine-tuned to steer the generation towards a broad range of property constraints.